

Science & Technology

REVIEW

July/August 2006

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

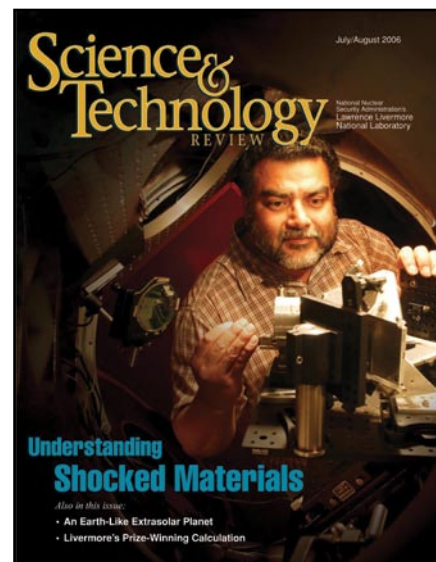
Understanding Shocked Materials

Also in this issue:

- An Earth-Like Extrasolar Planet
- Livermore's Prize-Winning Calculation

About the Cover

Using ultrabright, ultrafast x-ray sources at high-energy laser and accelerator facilities, Livermore scientists are directly measuring the x-ray diffraction and scattering that result from dynamic changes in a material's lattice. This effort, which is described in the article beginning on p. 4, will help researchers better understand how extreme dynamic stress affects a material's phase, strength, and damage evolution. Such information is essential to the Laboratory's work in support of the nation's Stockpile Stewardship Program. On the cover, Livermore physicist Hector Lorenzana aligns the target, detector, and laser beams in the vacuum chamber of the Laboratory's Janus laser for a dynamic x-ray diffraction experiment.



Photographer: Joseph Martinez

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str.



Prepared by LLNL under Contract
No. W-7405-Eng-48

© 2006. The Regents of the University of California. All rights reserved. This document has been authored by the Regents of the University of California under Contract No. W-7405-Eng-48 with the U.S. Government. To request permission to use any material contained in this document, please submit your request in writing to Library Report Orders, Lawrence Livermore National Laboratory, Mail Stop L-610, P.O. Box 808, Livermore, California 94551, or to our e-mail address report-orders@llnl.gov.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California and shall not be used for advertising or product endorsement purposes.

Contents

S&TR Staff

SCIENTIFIC EDITOR
Harry B. Radousky

MANAGING EDITOR
Ray Marazzi

PUBLICATION EDITOR
Carolyn Middleton

WRITERS
Arnie Heller, Ann Parker, Gabriele Rennie, and Maurina S. Sherman

ART DIRECTOR AND DESIGNER
Kitty Madison

COMPOSITOR
Louisa Cardoza

PROOFREADER
Pamela MacGregor

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the Web at www.llnl.gov/str.

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-06-7/8
Distribution Category UC-99
July/August 2006

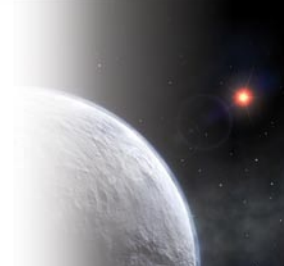
Features

- 3 Experiments at the Scale of Simulations**
Commentary by Tomás Díaz de la Rubia

- 4 A New Realm of Materials Science**
Livermore scientists are combining experiment, theory, and simulation to study the response of solids to extreme dynamic stresses at nanometer and subnanosecond scales.

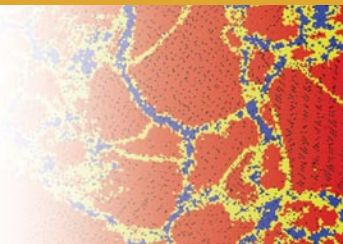


- 11 Planets and Stars under the Magnifying Glass**
An international collaboration involving Laboratory scientists has discovered a planet made of rock or ice orbiting a dim star outside our solar system.



Research Highlights

- 17 Keeping an Eye on the Prize**
A Livermore-IBM team uses a new code and the world's fastest computer to set a performance record for a science application.



Departments

- 2 The Laboratory in the News**
20 Patents and Awards
21 Abstracts

Shedding light on “ghost particles”

An international team of scientists, including Livermore physicists Peter Barnes, Doug Wright, and Ed Hartouni, announced that it has recorded the transformation of neutrinos from one type to another.

Neutrinos are particles with negligible mass and no electric charge yet are fundamental to the structure of the universe. Sometimes termed “ghost particles,” neutrinos are extremely difficult to detect because they rarely interact with anything. They come in three “flavors”: electron, muon, and tau. Each is related to a charged particle, which gives the corresponding neutrino its name.

The physicists have been working on the Main Injector Neutrino Oscillation Search (MINOS) Project, which was launched in 2005 to solve a 50-year-old mystery: how do neutrinos change flavors? MINOS uses two detectors, one located at the source of the neutrinos, at the Department of Energy’s Fermi National Accelerator Laboratory (Fermilab), in Batavia, Illinois, and the other located 725 kilometers away, at Soudan Underground Mine State Park in northern Minnesota.

A high-intensity beam of muon neutrinos generated at Fermilab traveled through Earth to the Soudan detector. Scientists observed that a significant fraction of these neutrinos disappeared, which indicates the muon neutrinos have changed to another kind—an effect known as neutrino oscillation. If neutrinos had no mass, the particles would not oscillate as they traverse Earth, and the MINOS detector in Soudan would have recorded many more muon neutrinos.

The findings, announced March 30, 2006, at Fermilab, will help scientists better understand how particles acquire mass, as well as neutrinos’ role in the formation of the universe and their relationship to dark matter.

Contact: Peter Barnes (925) 422-3384 (barnes26@llnl.gov).

Blue ring discovered around a giant planet

Earlier this year, scientists discovered two faint rings located well outside Uranus’s main ring system. The outer ring is centered on the orbit of the tiny moon Mab and is blue, while the other ring, which orbits between the moons Rosalind and Portia, is red.

Rings around the giant planets in our solar system—Jupiter, Saturn, Uranus, and Neptune—are typically reddish because they contain many large particles that mostly reflect longer (red) wavelengths of light. The only other known blue planetary ring is Saturn’s E ring, which hosts the moon Enceladus.

“We suspect that both rings owe their blue color to nongravitational forces acting on dust in the rings that allow

smaller particles to survive while larger ones are recaptured by the moons,” says Livermore scientist Seran Gibbard, who is a member of the research team. The team also includes Imke de Pater of the University of California at Berkeley, Mark Showalter of the SETI Institute, and Heidi Hammel of the Space Science Institute. The team’s research appeared in the April 7, 2006, issue of *Science*.

The blue ring was discovered by combining near-infrared observations from the Keck Telescope in Hawaii and visible-light photos taken by the Hubble Space Telescope. After other scientists discovered two new rings around Uranus, and two new moons, Mab and Cupid, the team reported seeing the red, innermost of the two new rings, but not the outermost. The outer ring could be seen in visible light but was not observable in the near-infrared, which indicates that it must be blue.

Contact: Seran Gibbard (925) 423-0656 (gibbard1@llnl.gov).

Pathogen informatics team contributes to SARS research

For the past six years, the pathogen informatics team in Livermore’s Biosciences Directorate has worked to find the genetic signatures of disease-causing microbes to help detect and diagnose human and animal pathogens. Recently, a Livermore-developed signature of the peculiar virus that causes severe acute respiratory syndrome (SARS) contributed to a landmark study of SARS in nonhuman primates. In the study, the U.S. Army Medical Research Institute of Infectious Diseases (USAMRIID) used the Livermore signature to detect the SARS virus in the body fluids of long-tailed macaque monkeys over a period of several weeks after they were infected. The research appeared in the May 2006 issue of *PLOS Medicine*.

The Livermore team began analyzing the SARS virus three years ago, after a sudden outbreak of the disease was reported in Asia. Using a map of the virus’s genome provided by the Centers for Disease Control and Prevention (CDC), the team of biologists, mathematicians, and computer scientists designed an initial set of potential virus signatures in just three hours. The team then used KPATH, a Laboratory-developed computational DNA signature design system, to produce 100 potential signatures. KPATH is a fully automated DNA-based signature “pipeline” that can deliver microbial signature candidates spanning 200- to 300-plus base pairs of DNA in minutes to hours. The CDC and USAMRIID later verified 3 of the 100 signatures in laboratory testing.

Contact: Thomas Slezak (925) 422-5746 (slezak@llnl.gov).



Experiments at the Scale of Simulations

TO advance our understanding of materials, especially when they are subjected to extreme conditions, Lawrence Livermore researchers are combining theory, experiments, and simulations in unprecedented ways. Our scientists and engineers are using the newest generation of the National Nuclear Security Administration's massively parallel supercomputers and codes based on first principles (the interactions between atoms) to generate atomistic simulations of material properties and performance at extremely short time and length scales. The data generated by these simulations allow scientists to develop a fundamentally new understanding of how materials respond to extreme temperatures and pressures.

Until recently, however, experimentalists could not carry out experiments at extreme conditions that simultaneously explored the length and time scales on which atoms move and the physics of the material response are controlled—that is, the scale of atomistic simulations. Typically, insights came from analyzing a material before and after it was subjected to extreme conditions. Scientists then inferred the governing phenomena from observations. Therefore, it was natural to ask: Are there ways in which we can experimentally probe these atomistic length and time scales simultaneously to both improve our understanding and validate our simulations?

As described in the article beginning on page 4, new techniques are allowing us to expand the amount of experimental information we can obtain on shocked materials at the same time and length scales used in simulations. The first technique, dynamic x-ray diffraction, requires high-intensity lasers to illuminate the changing microstructure of crystalline solids. For these experiments, researchers are using lasers at Lawrence Livermore and Los Alamos national laboratories, the University of Rochester, and Rutherford Appleton Laboratory in the United Kingdom.

The second technique, x-ray scattering, uses high-intensity x-ray sources generated by an accelerator light source, or synchrotron, to reveal defects and voids in microstructures. The Department of Energy's Office of Science is constructing the world's brightest

x-ray source, called the Linac Coherent Light Source, at the Stanford Linear Accelerator Center. We plan to take advantage of the facility when it is completed in 2009.

By using dynamic x-ray diffraction and scattering techniques, Livermore researchers for the first time will be able to directly compare the results of experiments and simulations. The researchers, funded by the Laboratory Directed Research and Development Program, are drawn from the Defense and Nuclear Technologies, Chemistry and Materials Science, National Ignition Facility (NIF) Programs, Engineering, and Computation directorates. We also have partnered with colleagues at other national laboratories and universities, including University of California campuses.

The new techniques will bring the experimentalist and computer scientist even closer together. Experiments allow us to plan and refine simulations, while simulations guide us to look for certain events in the results. Data gained from both approaches strengthen our theories and models.

This new era of experimental research is extremely important for the nation's stockpile stewardship program because material behavior is at the heart of most issues associated with this mission. In particular, scientists want to improve their ability to predict the effects of aging on weapon parts or the likely performance of remanufactured parts. The benefits of this research are certain to be much broader. For example, I expect that an important payoff will be for the NIF Programs, which plans to use the world's most energetic laser, located at Livermore, to explore the properties of materials driven to extreme conditions.

I also anticipate that we will further our understanding of how materials change phase, how defects in crystalline solids evolve, how a metal's microstructure changes in time, and how and why various materials fail. The result will yield important contributions to stockpile stewardship, materials science, industry, and basic scientific understanding.

■ Tomás Díaz de la Rubia is associate director for Chemistry and Materials Science.

A New Realm of Materials

A multidisciplinary approach to materials science provides insights on how solids respond to extreme dynamic stresses.

KNOWLEDGE is power, and for many scientists, understanding the dynamic lattice response of solids under extreme pressures, temperatures, and strain rates can be quite powerful, indeed. This quest to expand the fundamental knowledge of material behavior has spanned nearly a century, and it remains an exciting scientific frontier in high-energy-density materials science. Materials science is an essential part of Livermore's work in support of the National Nuclear Security Administration's Stockpile Stewardship Program to ensure the safety and reliability of the nation's nuclear weapons stockpile. In particular, scientists want to determine how extreme dynamic stress affects a material's phase, strength, and damage evolution.

Critical to this work are studies that probe material properties at the scale of the controlling physical processes—at length scales of 1 nanometer (10^{-9} meter) and time scales of less than 1 nanosecond (10^{-9} second). Investigations at these characteristic length and time scales were unthinkable a decade ago, but the technologies and facilities available today are bringing such studies within reach. Using ultrabright, ultrafast x-ray sources at high-energy laser and accelerator facilities, scientists can directly measure the x-ray diffraction and scattering that result from dynamic changes in a material's lattice.

A multidisciplinary team led by physicist Hector Lorenzana of the Laboratory's Defense and Nuclear Technologies Directorate is collaborating with researchers from other national laboratories and universities on a Laboratory Directed Research and Development (LDRD) project to probe the real-time lattice response of metals under high shock loads. The team's collaborators include researchers from Los Alamos, Argonne, Oak Ridge, and Lawrence Berkeley national laboratories as well as from Rochester University, Oxford University, Universidad Complutense de Madrid, and the University of Texas at Austin. The team's measurements, which have nanometer and subnanosecond resolutions, allow scientists to examine the fundamental mechanisms governing macroscopic behavior.

"Critical scientific questions about material response at the lattice level must be answered," says Lorenzana. "For our stockpile stewardship work, we are interested in characterizing the condensed-matter phase transformations and damage that occur in shocked solids. Working closely with the Laboratory's theoretical and computational experts, we are coupling the results of our experiments with first-principles simulations, which for the first time can explore physical phenomena at overlapping temporal and spatial scales."

Science



Livermore scientists Jim McNaney (left) and Hector Lorenzana check calibrations on the target chamber before a dynamic x-ray diffraction experiment.

Current Challenges and Obstacles

The measurement methodologies used to study dynamically compressed solids have been limited to large-scale probes such as time-resolved surface diagnostics or characterizations of recovered specimens. Such measurements limit scientists to three general time and length regimes: slow macro (slow time scales and macroscopic dimensions), slow micro, and fast macro. For example, slow macro techniques include Hopkinson bar mechanical testing. To study the slow micro regime, scientists can characterize the microstructure of shock-

recovered samples or observe materials compressed by a diamond anvil cell. With surface velocimetry or optical spectroscopy, they can probe the fast macro regime.

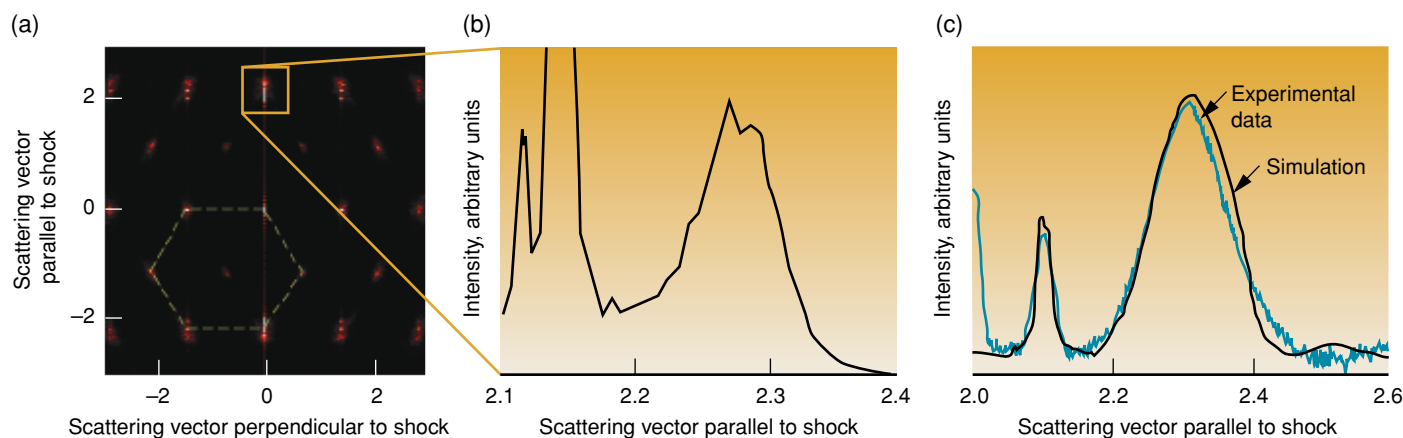
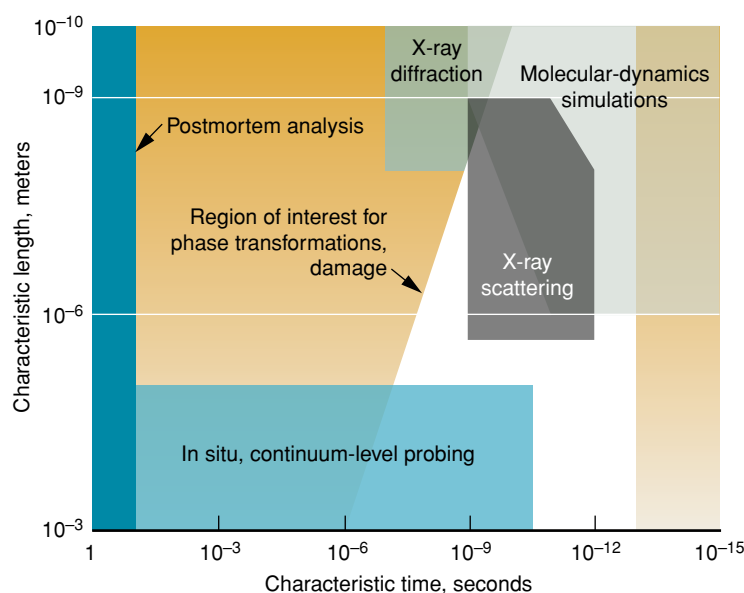
However, using these techniques, scientists must infer how physical processes interact at the atomic level under extreme shock loading. “To improve our understanding of the shocked solid, we must access the fast micro regime,” says Lorenzana. “For those studies, we need techniques that allow us to directly observe dynamic changes as they occur in a material’s lattice structure.”

Measurements in the fast micro regime can be used to characterize materials as they change phases, for example, as a solid melts or a material plastically deforms by creating a defected state. With such information, scientists can determine how damage evolves in a material under extreme pressures and causes the material to fail. “This next generation of fast micro probing will push our fundamental knowledge of shocked solids forward,” says physicist Bruce Remington, who works in Livermore’s National Ignition Facility (NIF) Programs Directorate, “and it will help us understand the microscopic lattice response under extreme conditions of compression. Research in the fast micro regime is important for achieving ignition on NIF, for example, where the target capsule’s response to the first shock can affect its subsequent implosion dynamics.”

Blending Experiment and Theory

Lorenzana emphasizes the importance of bridging experiment and theory at comparable temporal and spatial scales in the pursuit of new scientific discoveries. The LDRD project is the first comprehensive lattice-level study of the behavior of shocked solids using both experiments and simulations at overlapping length and time scales. “Experimental data allow us to quantify and validate our theories,” says Lorenzana. “Theoretical studies, in turn,

Few data are available to study the physical interactions that occur at very short time and length scales when materials are placed under extreme pressures. To examine this regime, scientists are combining new diagnostic techniques with computer simulations.



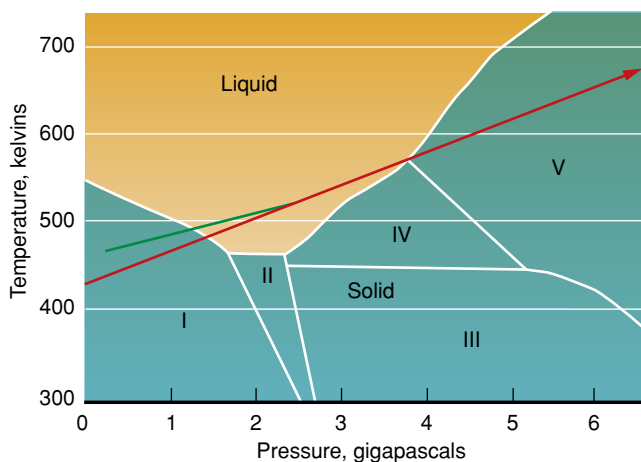
(a) Molecular-dynamics simulations of iron being transformed by shock predict the pattern of x-ray diffraction from many planes. (b) A closeup view of one lattice plane shows the predicted broadening and peak position of the diffraction signal. (c) The predicted response (black curve) from a simulation using a grain size of $8 \times 8 \times 8$ cells agrees with the experimental data (blue curve).

help us interpret the data and better design subsequent experiments. The outcome of this cycle is enhanced experiments and theory that lead us to an understanding of new physics.”

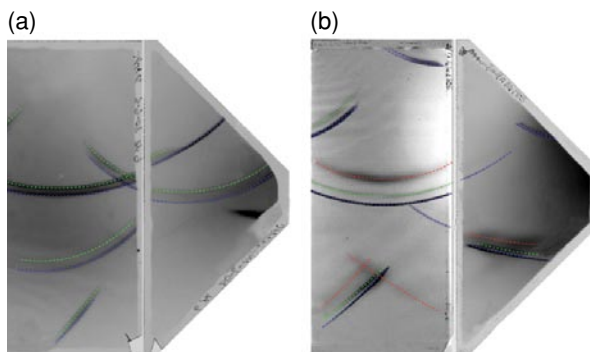
Also working on this project are Livermore physicists Eduardo Bringa, Babak Sadigh, and Jaime Marian of the Chemistry and Materials Science (CMS) Directorate. According to Bringa, the team’s work is providing a building block to improve scientific understanding of material behavior under dynamic loading, which is critical to the success of stockpile stewardship, energy research, and other important national endeavors.

“Livermore has some of the best computers in the world,” says Bringa. “With them, we can simulate systems atom by atom at the length and time scales used in our experiments and validate our materials models. In addition, the simulations provide detailed information about interactions that experiments cannot yet probe. Until we can develop experiments to study the evolution of shock-induced dislocation density with nanosecond resolution, we must rely on atomistic simulations to access such processes. Relevant information is lost in current recovered samples, where the unloading and thermal history greatly modify dislocation content.”

The metal bismuth illustrates the importance of unraveling material processes such as phase transformations. Bismuth exhibits a complex static phase diagram that presents challenges to researchers who study its solid-to-solid and solid-to-melt phase transformations during shock loading. At about 420 kelvins, shocked bismuth may melt and eventually resolidify as pressure is increased or released. According to Lorenzana, scientists want to predict how such phase transformations affect the material properties of the shocked solid, but they must first acquire accurate data on the changes that occur at the lattice level. Bismuth could serve as a test bed to study the kinetics of such transformations, allowing scientists to determine the rates of



A phase diagram of bismuth shows the material states that can occur as pressure and temperature vary. At about 420 kelvins, shocked bismuth may melt and resolidify as compression increases (red curve) or is released (green curve).



Micrographs from a dynamic x-ray diffraction experiment show the phase transformation in iron under extreme pressure: (a) at low pressure before transition and (b) at high pressure after the transition. Blue lines indicate the unshocked material. Green lines show the compressed phase of a material that is not transformed. Red lines show a new phase beginning to emerge.

phase changes and the location of phase boundaries.

Because damage prediction depends on a material’s microstructure and its phase history, scientists cannot predict a material’s response to shock loading until more questions are answered. “We must first address a broader series of open, fundamental physics questions,” says James McNaney, a materials scientist in the CMS Directorate. “For example, how is the microstructure modified under shock conditions? What are the dynamic high-pressure phases? How do molten and solid phases and the kinetics of the transitions affect the final state? And, perhaps most importantly, how does the resolidified material behave during subsequent loading?”

Directly measuring and simulating the response of an ordered crystalline solid to shock loading will go a long way toward answering these questions. “We are studying

key atomistic processes such as relaxation, phase transformation, and kinetics,” says Lorenzana. In addition, his team is looking at defect dynamics and evolution, including dislocations and the nucleation and growth of voids. (See the box on p. 8.)

Dynamic X-Ray Diffraction

A new diagnostic technique, called dynamic x-ray diffraction (DXRD), is providing great insight about the structure and spacing of the crystalline lattice in a shocked material. DXRD uses high-intensity lasers to generate both a shock in a solid and a precisely timed flash of x rays to image the lattice in motion. The x-ray flash can produce 100 to 1,000 times more photons per pulse than are produced by synchrotron accelerators. When the x rays interact with the crystal’s atoms, they are diffracted in a pattern that characterizes the lattice. This image is captured on x-ray

film. By resolving this time-dependent diffracted signal, scientists can develop a fundamental understanding of the kinetics of transformation and lattice relaxation.

In an effort to establish the effectiveness of the DXRD technique, a research team led by Livermore physicist Daniel Kalantar examined phase transformations in shocked iron. Materials scientists have frequently studied shock-compressed iron because the metal plays a key role in many important technologies and in the geophysical properties of Earth's formation. Despite the mature body of work associated with iron, no experiments had directly probed its lattice structure during shock loading. "In our DXRD experiments, we made the first direct observation of a

transition in iron," says Kalantar. "Now, we're experimenting with other materials and other configurations."

Lorenzana's team is expanding on these initial studies. "The feasibility studies with iron established the experimental and theoretical foundation for implementing DXRD methodologies," he says. "We look forward to investigating other important phenomena such as melting in bismuth and plasticity in vanadium."

To date, DXRD experiments have been conducted using the high-energy Janus laser at Livermore, the Trident laser at Los Alamos, the Omega laser at Rochester University, and the Vulcan laser at Rutherford Appleton Laboratory in the United Kingdom. "From a materials

science point of view, being able to study samples at the atomic level while they are being shocked opens up a new realm for us to investigate," says physicist James Hawreliak, a postdoctoral researcher working on Lorenzana's team. "Such studies under shock conditions are just scratching the surface of what we can learn."

X-Ray Scattering

An even newer technique is in the pipeline to probe these crystalline structures at superfast speeds and with high collimation. As with x-ray diffraction, scattering experiments require a high-intensity x-ray source directed at the crystal sample. Defects in the crystal lattice will cause the x rays to scatter, generating two types of

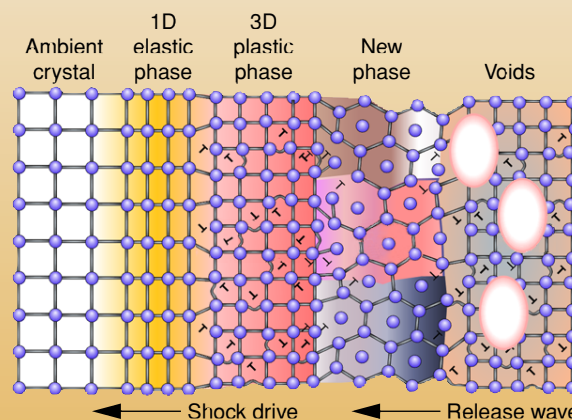
How Do Materials Behave under Shock?

Most metals are crystalline in nature—that is, they are solids composed of atoms arranged in a regularly ordered repeating pattern. When crystals form, they may solidify into either a polycrystalline solid or a single crystal. In a single crystal, all the atoms are arranged into one lattice or crystal structure. The structure of single crystals makes them ideal for studies of material response to shock loading.

When a highly ordered material, such as a metal crystal, is put under a planar shock, the crystal is compressed along the direction of the shock propagation. This uniaxial response can remain elastic so that, once the disturbance is removed, the lattice will relax back to its original configuration. However, under high-stress conditions, the configuration of atoms in the lattice may be changed irreversibly. Irreversible changes in phase and the development of defects at the atomic level lead to macroscopic changes, such as plasticity, melting, or solid-to-solid phase transformations. When the dynamic compression is removed, the shock-modified microstructure may influence the formation and growth of voids, cracks, and other processes that may cause the material to fail.

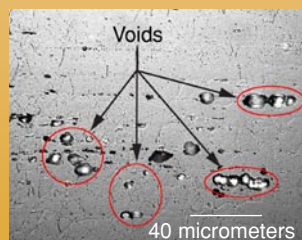
These atomistic changes can dramatically affect a material's behavior, such as its thermodynamic state, strength, and fracture toughness. Few

data are available on the phase transformations that occur under highly dynamic stress conditions or on the defects and voids that may form and grow as a result.



A crystal placed under shock loading will initially compress uniaxially and then relax plastically through defects (labeled with T's), a process known as the one-dimensional (1D) to three-dimensional (3D) transition. The material may also undergo a structural transformation, represented here as a cubic to hexagonal change. The transformation occurs over a characteristic time scale. The new phase may be a polycrystalline solid or melt. Once pressure is released, the microvoids that formed may grow, leading to macroscopic damage that causes the solid to fail.

This micrograph shows the voids that occur when a polycrystalline aluminum alloy is shocked and recovered. As the shock wave releases, the voids grow and may coalesce, resulting in material failure.



signatures: diffuse and small-angle scattering. Diffuse scattering can be used to examine atomic-scale defects in the crystal. Small-angle scattering allows scientists to characterize large-scale defects, particles, and voids.

"X-ray scattering studies have not been conducted under shock loading," says McNaney. The team plans to extend existing methodologies and analysis tools so scientists can use x-ray scattering to quantify damage in dynamically compressed materials.

"Small-angle x-ray scattering experiments with subnanosecond resolution are quite challenging because they combine extreme pressures, short time scales, and low signal-to-noise ratios," says Livermore physicist Anthony Van Buuren of the CMS Directorate. "Success in developing these techniques will allow us to study processes that must be understood to predict macroscopic behavior."

To bring this new experimental scheme into the regime needed to probe the shocked lattice response in situ, Lorenzana's team proposes to couple laser-based shock-generation techniques with the high brightness of an accelerator light source, or synchrotron, which can generate x-ray pulses that last about 100 picoseconds. X-ray scattering of the highly collimated and monochromatic beams produced by a synchrotron will provide data that can be analyzed to determine feature size, spacing, and morphology in the fast micro regime.

"Synchrotron radiation includes a large part of the electromagnetic spectrum—from infrared light to x rays," says team member Art Nelson, who works in the CMS Directorate. "In our measurements, we need a narrow band of x-ray wavelength, and on average, the synchrotron sources give more x-ray photons per pulse than conventional tabletop x-ray sources, such as diffractometers." In addition, these superbright, ultrafast x-ray pulses—as short as 70 femtoseconds—are highly collimated and can be focused to very small dimensions, making them ideal for looking at minute fluctuations in material

structures in the ultrafast time regimes. (See the box on p. 10.)

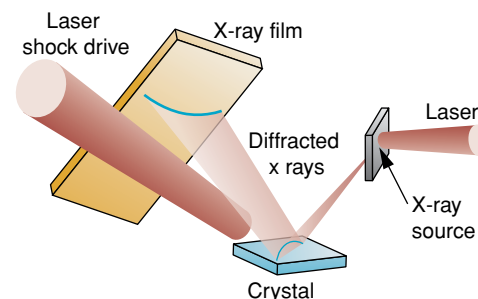
"Probing ultrafast phenomena is at the forefront of science," says Nelson, "not only in physics, but also in areas as diverse as chemistry and biology." For example, ultrafast biochemical processes such as photosynthesis are a potential area of inquiry that could benefit from superfast microscale probing. Says Nelson, "With these emerging methodologies, we can observe processes as they happen in nature."

Success So Far

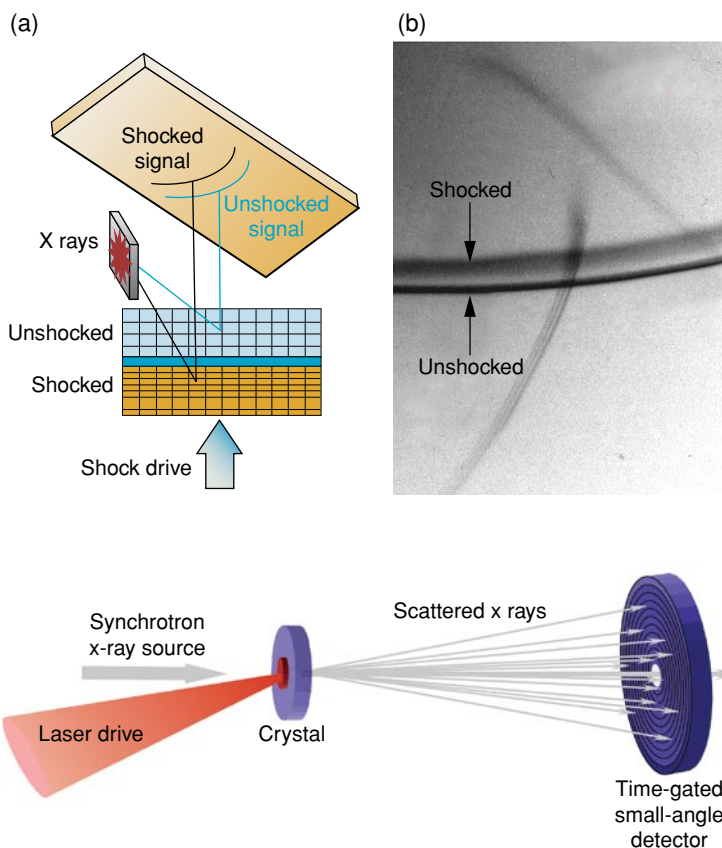
To date, the first-phase experiments have been performed on laser-based platforms at Livermore. Synchrotron-based investigations of shocked solids are planned for the latter part of 2006. Lorenzana acknowledges that much work is left to do. So far, the team is laying a technical foundation and demonstrating

proof of principle for in situ studies of lattice-level processes in shocked solids.

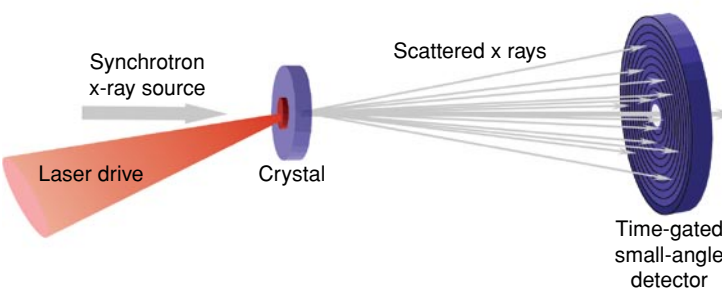
"We have demonstrated that our approach to probing highly dynamic shocked systems produces quantitative results at the physically relevant temporal and spatial scales," he says. "Success in this endeavor using laser- and synchrotron-based platforms will



Dynamic x-ray diffraction uses a high-intensity laser to shock a crystal sample. The x-ray diffraction pattern is recorded for later analysis.



Lattice compression shifts the x-ray diffracted signal in characteristic ways. (a) The change in lattice spacing will shift the angle of the diffracted arc, displacing the signal on the detector. (b) Measurements on titanium with Livermore's Janus laser clearly show the diffraction pattern.



X-ray scattering experiments using synchrotron accelerator light sources will allow scientists to measure the bulk distribution of material defects between 1 nanometer and 0.1 micrometer.

In Materials Science, Bright Is Might

Accelerator, or synchrotron, light sources, such as the Advanced Light Source at Lawrence Berkeley National Laboratory, provide the most brilliant x-ray beams available for scientific research. In these machines, electrons traveling at nearly the speed of light are forced into a circular path by magnets and emit bright radiation, from the infrared to the hard x ray, that shines down beam lines to experiment end stations. The x-ray light produced is one billion times brighter than that from the Sun.

The process begins by heating a cathode to more than 1,000°C. Electrons emitted from the cathode are accelerated first in a linear accelerator and then in a booster synchrotron. When the electrons reach the target speed, they are injected into a storage ring about the size of a football field. This ring uses a powerful electromagnetic field to focus the electrons into a narrow beam. During its orbit in the vacuum chamber, the electron beam is bent on a circular path. As the electrons circle the ring, they give off light that is called synchrotron radiation.

Synchrotron x rays have unique properties that make them ideal for dynamic materials science research, which involves fast time scales, microscopic length scales, and high collimation. Synchrotron sources produce more photons per pulse and brighter light than other x-ray sources. The light generated is a hundred million times brighter than that from the most powerful conventional x-ray tube.

An even brighter fourth-generation light source, the Linac Coherent Light Source, is under construction at the Stanford Linear Accelerator Center. Once it is operational, this x-ray free-electron laser will produce light that is hundreds to thousands of times brighter and shorter than the light from existing synchrotron-based x-ray sources. Single pulses will have enough photons to image diffraction patterns with femtosecond (10^{-15} -second) time resolution, providing an unmatched capability for investigating the material dynamics of shocked solids.



A multidisciplinary team of scientists drawn from several Livermore directorates is working together to better understand shock-compressed materials. Team members include (standing, from left to right) Daniel Kalantar, George Gilmer, Anthony Van Buuren, Jaime Marian, Bassem El-Dasher, James McNaney, Bruce Remington, and Santiago Casado and (sitting, from left to right) James Hawreliak, Babak Sadigh, Ben Torralva, Hector Lorenzana (team leader), and Eduardo Bringa.

position Livermore at the forefront of high-energy-density materials science.”

The successes from the shocked iron DXRD experiments have gone a long way in demonstrating a new ability to measure the lattice under shock conditions in previously unexplored regimes. This work, along with the real-time observation of phase transformations in situ, is breaking new ground beyond materials science and applications to nuclear weapons research. “The possibilities in these ultrafast, micro regimes are nearly limitless,” says Nelson. “Potential applications range from the genesis and characterization of new materials to probing any ultrafast process

that occurs in nature, such as biochemical processes that underlie human disease.”

In this case, accessing the fast micro regime is likely to mean huge scientific returns for a long time to come.

—Maurina S. Sherman

Key Words: crystalline lattice, dynamic x-ray diffraction (DXRD), materials science, phase transformations, shocked solids, ultrafast lattice response, x-ray scattering.

For further information contact
Hector Lorenzana (925) 422-8982
(lorenzana1@llnl.gov).

Planets and Stars under the Magnifying Glass

*Using the microlensing technique,
astronomers discover an Earth-like
planet outside our solar system.*

LOOKING out to the vastness of the night sky, stargazers often ponder questions about the universe, many wondering if planets like ours can be found somewhere out there. But teasing out the details in astronomical data that point to a possible Earth-like planet is exceedingly difficult.

To find an extrasolar planet—a planet that circles a star other than the Sun—astrophysicists have in the past searched for Doppler shifts, changes in the wavelength emitted by an object because of its motion. When an astronomical object moves toward an observer on Earth, the light it emits becomes higher in frequency and shifts to the blue end of the spectrum. When the object moves away from the observer, its light becomes lower in frequency and shifts to the red end. By measuring these changes in wavelength, astrophysicists can precisely calculate how quickly objects are moving toward or away from Earth. When

This artist's rendition shows the Earth-like extrasolar planet discovered in 2005. (Reprinted courtesy of the European Southern Observatory.)

a giant planet orbits a star, the planet's gravitational pull on the star produces a small (meters-per-second) back-and-forth Doppler shift in the star's light.

Using the Doppler-shift technique, astrophysicists have identified 179 planets within the Milky Way Galaxy. However, most of these are giant gas planets, similar in size to Jupiter and Saturn, and they orbit parent stars that are much closer to them than the Sun is to Earth. Planets similar in size to Earth have also been found, but they, too, are so close to their suns that they would be much hotter than Earth and too hot for life to exist.

In 2005, an international collaboration of astronomers working with telescope networks throughout the Southern Hemisphere uncovered clues to a small, rocky or icy planet similar to Earth. The new planet, designated OGLE-2005-BLG-290-Lb, is the farthest planet from our solar system detected to date. The discovery was made by the Probing Lensing Anomalies Network (PLANET) using microlensing—a technique developed nearly two decades ago by Livermore astrophysicists as part of the Massively Compact Halo Object (MACHO) Project, which searched for evidence of dark matter.

About the New Planet

According to Livermore astrophysicist Kem Cook, OGLE-2005-BLG-290-Lb is a low-mass planet. “It’s about 5.5 times the mass of Earth,” says Cook, who is a member of the PLANET collaboration. “The planet orbits a dim star about 390 million kilometers away from it, and one orbit takes about 10 years.” OGLE-2005-BLG-290-Lb is thus more than twice as far from its parent star as Earth is from the Sun. If the planet were in our solar system, it would be located between Mars and Jupiter. “It is the smallest extrasolar planet we’ve found orbiting a normal star,” Cook says, “and the most like Earth of any discovered so far.”

OGLE-2005-BLG-290-Lb orbits a faint red dwarf that lies about 22,000 light years from Earth, close to the center of the Milky Way Galaxy, in the constellation Sagittarius. Red dwarf stars are relatively cool, stellarly speaking. Temperatures on the planet would thus be similar to those on Neptune or Pluto—about -220°C , too cold for liquid water or even liquid oxygen, which freezes at -219°C . “The planet must be made of rock or ice,” says Cook. “Its mass is too small to have been formed of only gas, so we can discount that it’s a gaseous planet.”

This discovery joins a relatively short lineup of planets identified so far. “When

we consider the number of stars out there,” Cook says, “the fact that we stumbled on one small planet means that thousands more are waiting to be found.”

Detection through Microlensing

The concept of microlensing took root in the fertile mind of none other than Albert Einstein. In 1936, Einstein published a paper in *Science* on a theory involving what might occur to the observed light from a star (star A) if another star (star B) were directly in the line of sight between an observer on Earth and star A. Einstein showed that when the two stars are exactly aligned with the observer, a ringlike image forms. If star B moves a small distance from the line of sight, the observer will see two images of star A.

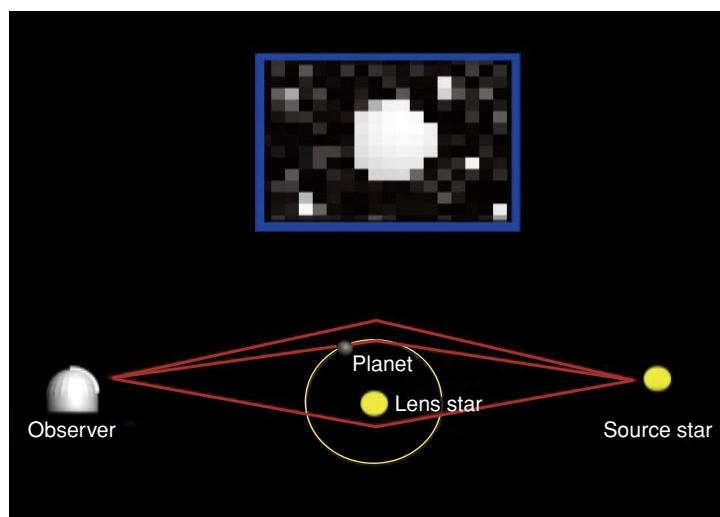
Because of the geometry of microlensing, the observer would not be able to resolve either the ringlike image or the double images. Instead, star A would appear to brighten because the total luminosity of the two images or ring would be greater than the luminosity of star A by itself. This brightening is caused by the microlensing effect in which star B’s gravity acts as a gravitational lens, bending the light from star A around star B and focusing it toward the observer.

Scientists can distinguish microlensing from other phenomena that lead to brightening, such as a flare or a variable star. A microlensing light curve is well defined, and the lensing effect is wavelength independent. Another distinction is that the microlensing event for a star does not repeat. If a second brightening appears before or after the peak in amplification, the so-called bump is probably caused by a variable star. A planet orbiting the closer (lensing) star will also modify the lensing effect, adding a spike of brightness to the otherwise smooth magnification curve.

MACHO Started It All

Although Einstein proposed the possibility of microlensing, astronomers

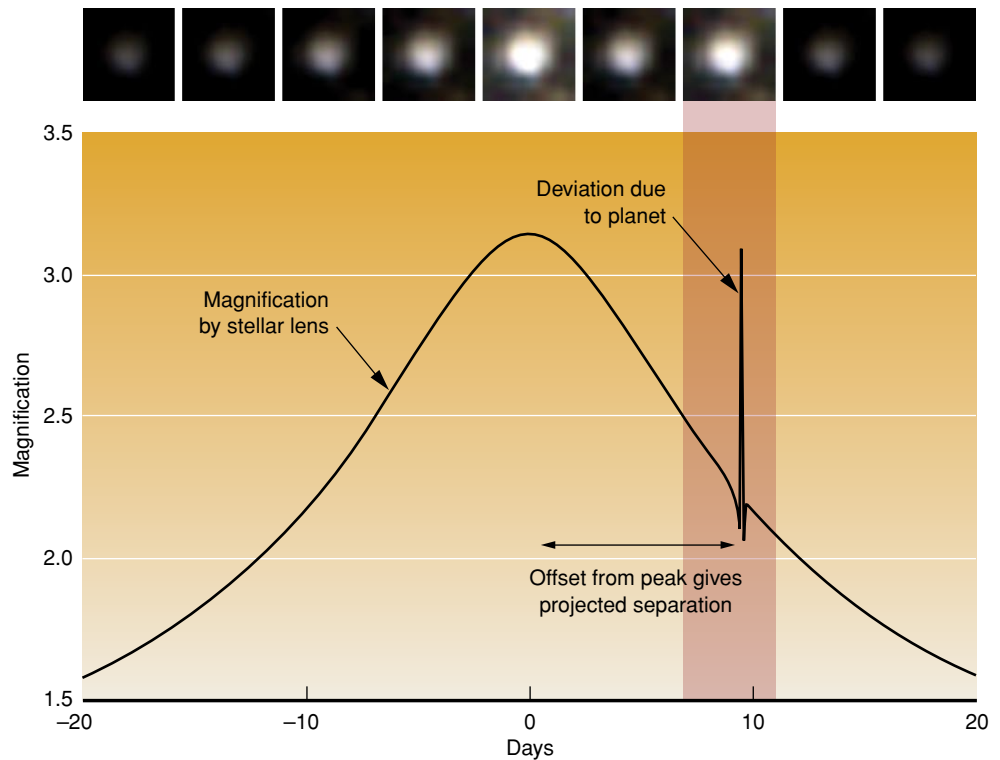
Gravitational microlensing (top box) occurs when light from a source star is bent and focused by gravity as a second object (the lens star) passes between the source star and an observer on Earth. A planet rotating around the lens star will produce an additional deviation in the microlensing.



did not have the technology to observe the effect for more than 50 years. According to Cook, such observations became feasible in the late 1980s when new imaging techniques were developed for the Strategic Defense Initiative (SDI). President Ronald Reagan established SDI in 1983 to develop ground- and space-based systems to protect the U.S. from attack by strategic nuclear ballistic missiles. Scientists working on SDI were asked to find methods to observe a large area of sky in search of incoming objects. "These systems required wide-field-of-view cameras that could record a slice of the sky over time and imaging software to interpret the data," says Cook. "Once these technologies were available, astronomers began to apply them to their own field."

In 1987, Livermore astrophysicist Charles Alcock, who is now the director of the Harvard-Smithsonian Center for Astrophysics, wanted to apply this imaging technology to search for comets at the outer edge of the solar system. He had read a 1986 scientific paper written by Bohdan Paczynski, an astrophysicist then at Princeton University, proposing the use of gravitational microlensing to identify MACHOs. Alcock realized a new technology, the large-format charge-coupled device (CCD), was sensitive enough to detect the tiny increase in brightness that occurs when a massive object passes in front of and microlenses a star.

Alcock, Cook, and Livermore physicists Tim Axelrod and Hye-Sook Park formed a team to study this application. The scientists did not work with actual SDI equipment. Rather, they considered possible designs for a system that used SDI technology to produce many thousands of digital images from the night sky, reduce the data, and interpret the results. In 1989, Livermore's Laboratory Directed Research and Development Program funded the MACHO Project, and design work began in earnest. The MACHO team created an optical imaging system with an exceptionally wide



Data from a microlensing event indicate a smooth, symmetric magnification curve as a lens star moves between a source star and an observatory on Earth. The short spike in magnification is caused by a planet orbiting the lens star.

field of view and a large detector. The area imaged by the system was about 10 times larger than the area covered by telescopes in operation at that time.

As work progressed, astronomers outside the Laboratory began to take interest in the possibilities offered by the new system. Several organizations, including the University of California's Center for Particle Astrophysics, began a search to find a location suitable for building a telescope and devoting research efforts to the MACHO Project. The potential site had to offer a clear view of the Large Magellanic Cloud (LMC), a neighboring galaxy that is visible from the Southern Hemisphere. The Australian National University agreed to dedicate its 1.27-meter reflecting telescope at the Mount Stromlo and Siding Spring Observatories to the MACHO Project for four years. The

first optical imaging system to fully exploit the new generation of large-format CCD images was installed on this telescope.

The MACHO Project has evolved into a second-generation sky survey called SuperMACHO, which uses the National Science Foundation's Victor M. Blanco 4-meter telescope at Cerro Tololo Inter-American Observatory in Chile. The SuperMACHO team, which includes Cook and Livermore scientists Sergei Nikolaev and Mark Huber, is searching for signs of microlensing by MACHOs between stars in the LMC and Earth. The team's goal is to determine what causes a large number of reported microlensing events toward the LMC.

The MACHO Project also served as a prototype for other collaborative sky surveys, including the Optical Gravitational Lensing

Experiment (OGLE) and Microlensing Observations in Astrophysics (MOA). The OGLE survey, a Polish collaboration that began in 1992, focused on microlensing toward the bulge of the galaxy. The first OGLE campaign used the Henrietta Swope 1-meter telescope operated by the Las Campanas Observatory in Chile and ran through four observing seasons. In its second campaign, which began in 1997, the OGLE team used a 1.3-meter telescope to survey the Magellanic Clouds and Galactic Bulge. Now in its third campaign, OGLE regularly monitors 120 million stars and, from these data, identifies hundreds of

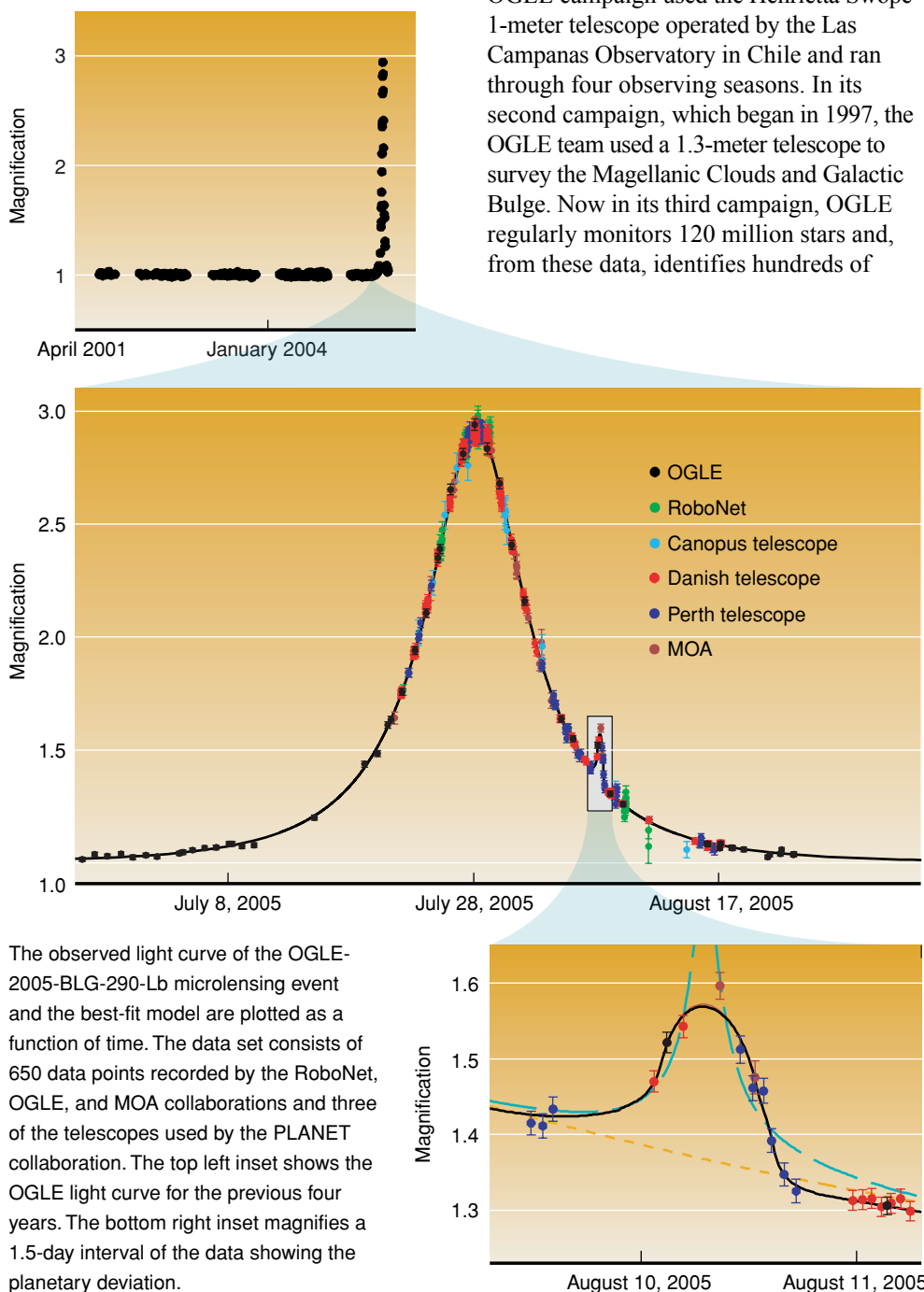
microlensing events per observing season. In the 2005 season, the team observed about 600 microlensing candidates.

Telescopes on the Prowl

The OGLE team's success in identifying candidate events rests in part on its automatic early-warning system, which analyzes image data in real time. The warning system's software measures the light intensity of all the stars in each image. If a star's intensity differs in three consecutive images, the system flags that star for further analysis. Astronomers then visually inspect the recorded light curves of flagged stars. They also check each star's position on recent CCD frames to ensure that changes in brightness are not caused by bad pixels or bright neighboring stars.

If a star passes the checks, the survey team announces it as a microlensing candidate to the observation networks. Alerts are posted on survey project Web sites, and e-mail announcements are sent to interested parties. Networks of telescopes are then programmed to provide round-the-clock coverage, and like runners handing off a baton in a relay race, telescope stations pass monitoring activities from one telescope to the next as an event moves through its cycle.

Microlensing events typically last for 15 to 90 days. Survey teams such as OGLE produce light curves that are sampled about once per day. The brightening caused by an intervening star usually lasts about a month—long enough to be visible in data recorded on this time scale. More precise resolution is required to capture the faint, elusive signal that heralds a planet. The planetary brightening may last a few days for a giant planet or only a few hours for one the size of Earth. Detecting a planet thus requires quick, highly precise data collection 24 hours a day. Sampling on these shorter time scales must be done separately. Scientists on the PLANET team and their partners at the United Kingdom's Robotic Telescope Network (RoboNet) train



The observed light curve of the OGLE-2005-BLG-290-Lb microlensing event and the best-fit model are plotted as a function of time. The data set consists of 650 data points recorded by the RoboNet, OGLE, and MOA collaborations and three of the telescopes used by the PLANET collaboration. The top left inset shows the OGLE light curve for the previous four years. The bottom right inset magnifies a 1.5-day interval of the data showing the planetary deviation.

PLANET Formation

Astronomy centers began to establish microlensing collaborations in the early 1990s to build on the success of surveys conducted by the Massively Compact Halo Object (MACHO) Project. Collaborations such as the Optical Gravitational Lensing Experiment (OGLE) provide networks of telescopes to track microlensing events on long time scales. These microlensing survey teams record data at intervals of 1 to 5 days. Sampling at shorter time scales, for example, once a day or every hour, is done separately by collaborations such as the Probing Lensing Anomalies Network (PLANET).

Established in 1995, PLANET is an international collaboration that provides astronomers with access to Dutch, South African, and Australian telescopes. PLANET's primary goal is to study the anomalies found in the light curves of microlensing events. Not all of these indicate the presence of a planet—many astronomical events can cause deviations in microlensing data. For example, the source star may be so large that the lens star magnifies only part of it at one time, or light from other stars may blend with amplified light along an event's line of sight. Another common anomaly occurs when two lenses are so close to each other that their magnification patterns overlap, an effect called binary lensing.

Detailed data recorded over short sampling times provide the clues needed to differentiate these anomalies. Therefore, when a microlensing candidate is announced, one or another of PLANET's telescopes is focused on the target area 24 hours a day. The PLANET network of 1-meter-class telescopes consists of the European Southern Observatory's 1.54-meter Danish telescope at La Silla in Chile, the Mount Canopus Observatory's 1.0-meter telescope in Australia, the Perth Observatory's 0.6-meter telescope in western Australia, the Boyden Observatory's 1.5-meter telescope in South Africa, and the South African Astronomical Observatory's 1.0-meter telescope. In 2005, PLANET joined forces with the Robotic Telescope Network (RoboNet), which is operated by the United Kingdom. RoboNet has 2-meter fully robotic telescopes, one in Spain and the other in Hawaii.

The MACHO Project completed its survey in 2000. OGLE continues to find 500 to 600 microlensing events annually and sends alerts to other telescope networks, such as PLANET. "The Polish system is positively spewing out microlensing events," says Livermore astrophysicist Kem Cook, who is a member of the PLANET collaboration. "MACHO, even at its peak, recorded about 100 events a year." The large number of microlensing alerts keeps PLANET telescopes busy from May through September, when the Galactic Bulge is visible in the Southern Hemisphere.

The PLANET/RoboNet collaboration uses telescopes throughout the Southern Hemisphere, including the 1.5-meter telescope at the Boyden Observatory in South Africa. (Reprinted courtesy of the Boyden Observatory.)



their telescopes on identified sections of the sky and record data on the finer time scale.

Confirming the discovery of OGLE-2005-BLG-290-Lb involved four survey teams: PLANET/RoboNet, OGLE, MOA, and an informal consortium called MicroFUN (the Microlensing Follow-up Network). Scientists working on the OGLE collaboration first detected the home star of the planet on July 11, 2005. Once the microlensing event was announced, the PLANET/RoboNet collaboration, which included Livermore scientists, used a network of telescopes in the Southern Hemisphere to survey the targeted section of the Galactic Bulge in the Milky Way. (See the box on p. 15.) A tiny change in the microlensing light curve, signaling a possible planet, was observed on August 10, 2005, from PLANET's Chilean telescope in La Silla and was noted in light curves recorded by the Perth Observatory in Australia. The additional brightening was about 15 percent of the total light recorded and lasted for

only 12 hours. The MOA survey team later identified the microlensing event on its images and confirmed the deviation. The planet's discovery was announced in a letter published in the January 26, 2006, issue of *Nature*. Altogether, the six-month effort involved 73 collaborators affiliated with 32 institutions in 12 countries.

More Planets in the Offing?

The small, frozen planet has planetary scientists taking note. A popular model of planetary formation suggests that red dwarf stars should be likely suns for Earth- to Neptune-mass planets with orbits up to 10 times greater than Earth's orbit of the Sun. The discovery of OGLE-2005-BLG-290-Lb supports this theory. "It's not an exaggeration to say that the discovery opens a new chapter in the search for planets that could support life," says Cook.

The collaboration continues, with the observing networks on call to monitor microlensing alerts for evidence of other

planets. In the future, astrophysicists hope a microlensing detection system can be launched in space. "That would be the ideal situation," Cook says. "With a system in space, we could avoid the problems of weather and atmospheric distortion. So perhaps one day, we'll be able to move the search for planets away from Earth."

—Ann Parker

Key Words: extrasolar planets, gravitational microlensing, Massively Compact Halo Object (MACHO) Project, Microlensing Observations in Astrophysics (MOA), OGLE-2005-BLG-290-Lb, Optical Gravitational Lensing Experiment (OGLE), Probing Lensing Anomalies Network (PLANET), Robotic Telescope Network (RoboNet).

For further information contact Kem Cook
(925) 423-4634 (cook12@llnl.gov).

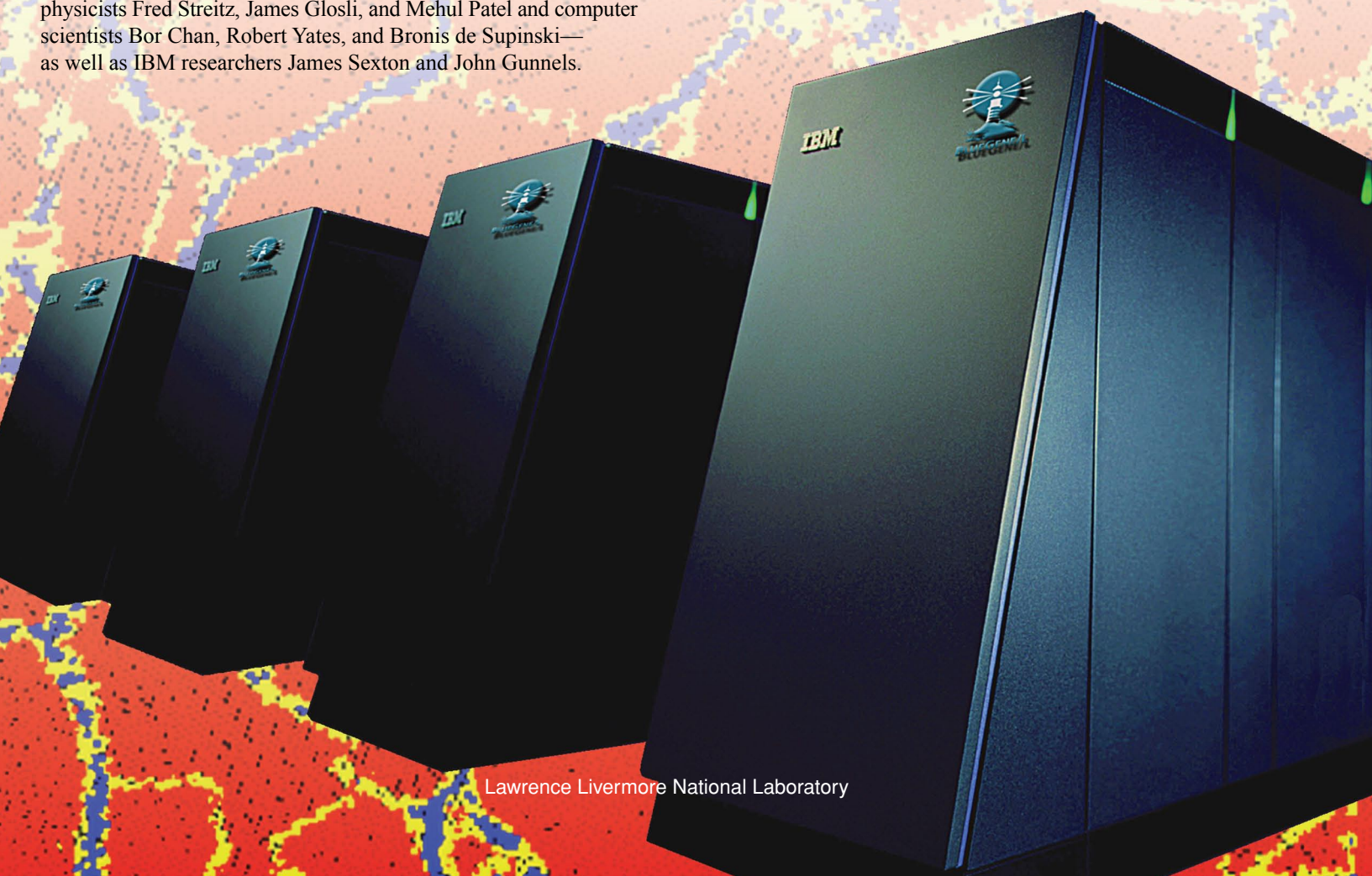
Keeping an Eye on the Prize

SETTING performance goals is part of the business plan for almost every company. The same is true in the world of supercomputers. Ten years ago, the Department of Energy (DOE) launched the Accelerated Strategic Computing Initiative (ASCI) to help ensure the safety and reliability of the nation's nuclear weapons stockpile without nuclear testing. ASCI, which is now called the Advanced Simulation and Computing (ASC) Program and is managed by DOE's National Nuclear Security Administration (NNSA), set an initial 10-year goal to obtain computers that could process up to 100 trillion floating-point operations per second (teraflops). Many computer experts thought the goal was overly ambitious, but the program's results have proved them wrong.

Last November, a Livermore-IBM team received the 2005 Gordon Bell Prize for achieving more than 100 teraflops while modeling the pressure-induced solidification of molten metal. The prestigious prize, which is named for a founding father of supercomputing, is awarded each year at the Supercomputing Conference to innovators who advance high-performance computing. Recipients for the 2005 prize included six Livermore scientists—physicists Fred Streitz, James Glosli, and Mehul Patel and computer scientists Bor Chan, Robert Yates, and Bronis de Supinski—as well as IBM researchers James Sexton and John Gunnels.

This team produced the first atomic-scale model of metal solidification from the liquid phase with results that were independent of system size. The record-setting calculation used Livermore's domain decomposition molecular-dynamics (ddcMD) code running on BlueGene/L, a supercomputer developed by IBM in partnership with the ASC Program. BlueGene/L reached 280.6 teraflops on the Linpack benchmark, the industry standard used to measure computing speed. As a result, it ranks first on the list of Top500 Supercomputer Sites released in November 2005.

To evaluate the performance of nuclear weapons systems, scientists must understand how materials behave under extreme conditions. Because experiments at high pressures and temperatures are often difficult or impossible to conduct, scientists rely on computer models that have been validated with obtainable data. Of particular interest to weapons scientists is the solidification of metals. "To predict the performance of aging nuclear weapons, we need detailed information on a material's phase transitions," says Streitz, who leads the Livermore-IBM team. For example, scientists



want to know what happens to a metal as it changes from molten liquid to a solid and how that transition affects the material's characteristics, such as its strength.

A New Code for Complex Systems

One metal the team simulated was the transition metal tantalum. In transition metals, the valence electrons, which interact with other elements to form compounds, are present in more than one shell. Thus, as tantalum solidifies, complex bonding structures form, and the transition from a melt phase to a solid can happen very slowly. These physical processes are challenging to model. A simulation of tantalum solidification may require billions of atoms, and the code must run many millions of time steps even though the process being simulated may last no more than a few nanoseconds.

Researchers have been modeling systems with billions of atoms for about 10 years. However, these models rely mainly on pair-potential techniques to describe the force each atom exerts on every other atom. Pair-potential techniques are effective for simple systems, such as those involving noble gases. Because noble gases have closed shells of electrons, the forces exerted on the atom are radially symmetric, resulting in spherically symmetric bonds.

Pair-potential techniques do not model complex systems with the accuracy needed for stockpile stewardship research. Most of the transition metals—including tantalum—contain a partially filled d band of electrons, which results in a more complicated bonding structure. For example, forces exerted on atoms are angularly dependent, and bonds may form between three or four atoms in a surrounding area. Accurately modeling these forces requires a sophisticated interaction potential.

In 1990, Livermore physicist John Moriarty developed the model-generalized pseudo-potential theory (MGPT), which can be used to

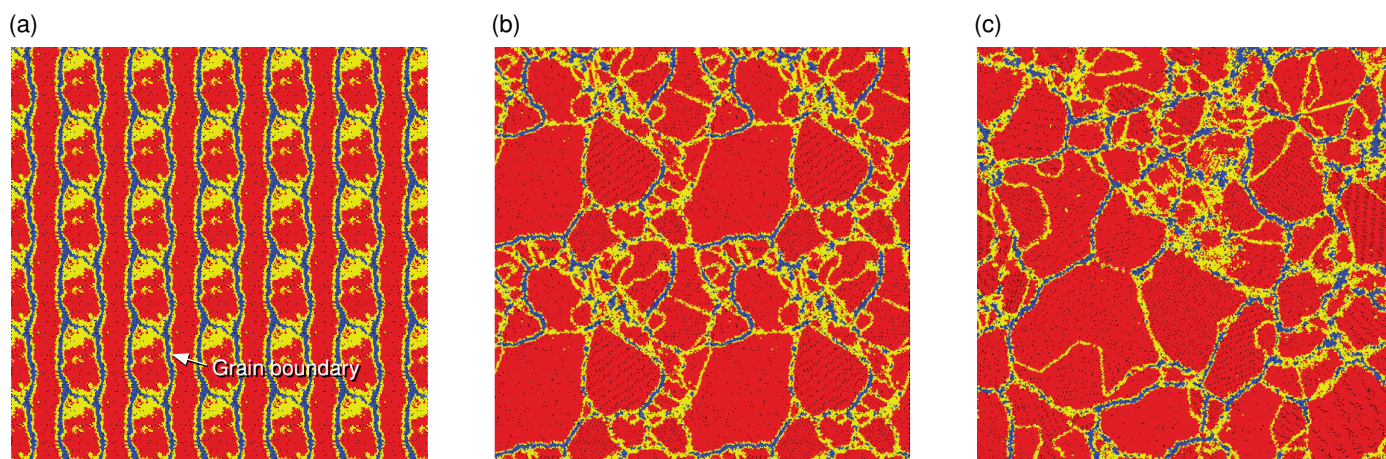
derive more accurate quantum-based interaction potentials. MGPT potentials are based on many-body expansions of a quantum-mechanically derived energy surface and include terms for two-, three-, and four-atom bonds. These potentials are validated by comparing information obtained by first-principles calculations and experiments.

Streitz and Patel first used MGPT potentials in 2000 in a single-processor code they had developed to model metal solidification. In 2002, Glosli joined the team, restructuring the MGPT potential routine and increasing single-processor performance by a factor of 20. He quickly became the principal architect of what is now the ddcMD code, leading the design and implementation of a novel domain decomposition algorithm that enabled parallel processing.

In the first full machine run on BlueGene/L, the team clocked the ddcMD code at 75 teraflops, significantly close to the ASC goal of 100 teraflops on a production science code. By focusing on the small matrix-matrix multiplication routines at the heart of the MGPT potentials, Glosli, Chan, and Gunnels boosted performance on short benchmark simulations to more than 107 teraflops. During a 7-hour production science run using all 131,072 processors, the team measured ddcMD performance at 101.7 teraflops—the highest sustained performance of a scientific application code.

Integrated Design a Major Advantage

The major difference between BlueGene/L and other computers is its scalability, which is provided by a large number of low-power processors and multiple integrated interconnection networks. BlueGene/L has 65,536 nodes, compared with 512 nodes for Livermore's ASC White machine, 1,536 for Purple, and 2,048 for the Q machine at Los Alamos National Laboratory. To accommodate this large number of nodes, IBM designed BlueGene/L with a simple



The Livermore-IBM team used three system sizes to simulate the transition of tantalum from a melt to a solid. (a) With a 64,000-atom system, the simulation produced an artificial grain-boundary pattern. (b) A simulation with more than 2 million atoms yielded a more realistic but restricted grain-size distribution. (c) The result from using 16 million atoms showed grain formation and growth independent of system size.

architecture that includes only 10 chips per node: nine memory chips and one compute application-specific integrated circuit (ASIC) chip. In comparison, a desktop computer can have 50 to 60 individual chips. The ASIC is a complete system-on-a-chip. It includes two IBM PowerPC 440 processors and five interconnects, and it provides 8 megabytes of embedded dynamic random access memory.

BlueGene/L's highly integrated design scales up in an orderly fashion with relatively modest power and cooling requirements. In 2004, when BlueGene/L assumed the number 1 spot on the Top500 list, it did so with only one-quarter of the final system, clocking 70.72 teraflops. (See *S&TR*, April 2005, pp. 23–25.) BlueGene/L beat the previous record holder, Japan's Earth Simulator, by a factor of two.

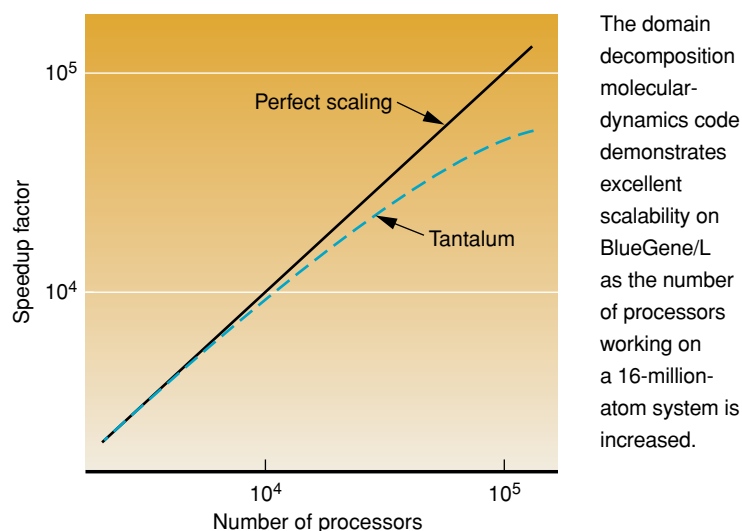
With the ddcMD code running on BlueGene/L, weapons scientists can simulate billions of atoms on the necessary time scales to obtain reliable results. "Prior to BlueGene/L, the added computational expense of the potentials we needed for the tantalum studies would have limited us to about 10,000 atoms for a 1-nanosecond simulation," says Streitz. "Not only would that calculation have taken a month to run, but the system being simulated would still be about 20 times smaller in size than what we need to access the required physics."

For the molten tantalum studies, the team modeled systems ranging from 64,000 to 128 million atoms compressed to 250 gigapascals of pressure at 5,000 kelvins. By varying the size of a simulation, the researchers gained confidence that their results were not affected by the size of the system being modeled. The 64,000-atom simulation showed two large grains, with a grain boundary spanning the simulation cell—an unrealistic result that indicated the system size was too small. In the simulation with more than 2 million atoms, the distribution of grain sizes was much more realistic. When the model size reached 16 million atoms, grain formation and growth were completely independent of system size. These simulations are the first step toward modeling nucleation—when the transition to the solid phase begins—and growth in a manner that allows scientists to directly link processes at atomistic scales to those at micrometer scales and above.

Doesn't Skip a Beat with Added Load

With many high-performance codes, increasing the number of processors will eventually slow computing performance substantially because the processors need more time to communicate with each other. In contrast, the ddcMD code can achieve excellent scaling performance on BlueGene/L because of the algorithms that Glosli incorporated into the code. It maintains almost perfect scalability even as the number of processors is increased from less than 1,000 to more than 100,000.

This scalability also allows researchers to adjust the system size to extract specific information. "Although a 64,000-atom system is too small for modeling molten tantalum through to its solid phase, the nucleation event may be the same in the small system as it is in



a 16-million-atom system," says Streitz. "We can glean valuable data even from smaller system sizes."

The team is sifting through the information produced by the solidification simulations on BlueGene/L. "We have a mammoth amount of data that we still need to go through," says Glosli. "We may find some surprises in the results."

Long-Term Goals Pay Off

The team's simulations will help scientists develop larger-scale models of material behavior. They also are providing more information about the nucleation and growth processes that occur during solidification and how factors such as temperature and strain rate affect these processes. "Ultimately," says Glosli, "we want to build models that reduce processor time even further."

Surpassing 100-plus teraflops using a scientific application marks an important milestone for supercomputing. The simulations of metal solidification are providing valuable insight for NNSA's stockpile stewardship efforts to ensure the safety and reliability of the nation's nuclear deterrent. The acknowledgment of this record-setting achievement by the Gordon Bell Prize demonstrates that BlueGene/L can deliver as promised.

—Gabriele Rennie

Key Words: Accelerated Strategic Computing Initiative (ASCI), Advanced Simulation and Computing (ASC) Program, BlueGene/L, domain decomposition molecular-dynamics (ddcMD) code, Gordon Bell Prize, model-generalized pseudo-potential theory (MGPT), solidification.

For further information contact Fred Streitz (925) 423-3236 (streitz1@llnl.gov).

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Low Power Integrated Pumping and Valving Arrays for Microfluidic Systems

Peter A. Krulevitch, William J. Benett, Klint A. Rose, Julie Hamilton, Mariam Maghribi

U.S. Patent 7,025,323 B2

April 11, 2006

Low-power integrated pumping and valving arrays provide a new approach for performing these operations in microfabricated fluidic systems, such as the microchips used in medical diagnostics. Traditional methods that rely on external high-pressure sources do not offer the advantages of miniaturization. Other microfabrication devices are power and voltage intensive and, thus, only function at sufficient pressure to be broadly applicable. This new approach integrates a lower power, high-pressure source with a polymer, ceramic, or metal plug enclosed within a microchannel, analogous to a microsyringe. When the pressure source is activated, the polymer plug slides within the microchannel, pumping the fluid on the opposite side of the plug without allowing fluid to leak around the plug. The plugs also can serve as microvalves.

Solid-Water Detoxifying Reagents for Chemical and Biological Agents

Dennis M. Hoffman, Ing Lap Chiu

U.S. Patent 7,030,071 B2

April 18, 2006

Solid-water reagents for detoxifying chemical and biological agents are formed by coating reagent solutions with small quantities of hydrophobic nanoparticles. When the aerosolized solution is shaken vigorously in the presence of the nanoparticles, a solid powder forms. For example, when hydrophobic fumed silica particles are shaken in one normal concentration of Oxone in aqueous solution at a ratio of about 95 to 5, the silica forms

a porous coating of insoluble fine particles around the solution. Chemical and biological agents tend to be hydrophobic. Therefore, when the weakly encapsulated detoxifying solution contacts an agent, the porous coating breaks down. The detoxifying reagent is then delivered directly to the chemical or biological agent, providing maximum concentration at the point it is needed. The solid-water (coated) solution can be blown into contaminated ventilation ducting or other difficult-to-reach sites to detoxify pools of a chemical or biological agent. Once an agent has been detoxified, it can be removed by flushing the area with air or other techniques.

Laser Driven Ion Accelerator

Toshiki Tajima

U.S. Patent 7,030,398 B2

April 18, 2006

This system for accelerating ions optimizes the energy produced by a light source. With the system, an accelerator's performance can be adjusted by controlling different parameters when constructing the accelerator target, such as the target's material, thickness, geometry, and surface.

Electronic Unit Integrated into a Flexible Polymer Body

Peter A. Krulevitch, Mariam N. Maghribi, William J. Benett, Julie K. Hamilton, Klint A. Rose, James Courtney Davidson, Mark S. Strauch

U.S. Patent 7,030,411 B2

April 18, 2006

This peel-and-stick electronic system has a silicone body with at least one electronic unit connected to it. The electronic system is produced by providing a silicone layer on a substrate, providing a metal layer on the silicone layer, and providing at least one electronic unit connected to the metal layer.

Awards

The **Federal Laboratory Consortium for Technology Transfer** (FLC) honored a team of Livermore scientists with an **Excellence in Technology Transfer Award** for developing a portable explosives detector called the Easy Livermore Inspection Test for Explosives (ELITE). Team members include **John Reynolds**, the team leader and deputy director of the Laboratory's Forensic Science Center; engineer **Del Eckels**; chemists **Peter Nunes**, **Rich Whipple**, **Phil Pagoria**, and **Marina Chiarappa-Zucca**; and chemist **Randy Simpson**, who also serves as director of Livermore's Energetic Materials Center. The two centers partnered on the ELITE project, which was sponsored by the Department of Energy (DOE) and the National Nuclear Security Administration (NNSA). ELITE has been licensed to Field Forensics, Inc., in St. Petersburg, Florida, and was placed on the market in October 2005.

A nationwide network of federal laboratories, FLC provides a forum to develop strategies and opportunities for linking the laboratory mission technologies and expertise with the marketplace. Organized in 1974 and formally chartered by the Federal Technology Transfer Act of 1986, FLC consists of

more than 700 federal laboratories and centers and their parent departments and agencies.

Laboratory Classification and Export Control Officer **Dave Brown** received a **Certificate of Excellence** from DOE's **Office of Classification, Office of Security and Safety Performance Assurance**. Brown was honored because his "outstanding leadership has enabled [his] staff to accomplish expert reviews of massive numbers of documents, year after year, for a host of customers, responding to the needs of the nuclear weapons community while building trust with environmental, safety and health advocates."

Brown also received an **Award of Excellence** from DOE's **Defense Program** for his contribution to the Stockpile Stewardship Program and a plaque from **NNSA** "for dedicated leadership and technical expertise." Brown has worked at the Laboratory for 21 years and has served as Classification Officer for the past 8 years. In addition, for 2 years, he chaired the national Weapons Contractor Classification Conference.

A New Realm of Materials Science

A multidisciplinary team of Lawrence Livermore scientists is collaborating with researchers from other national laboratories and universities on a Laboratory Directed Research and Development project to study material behavior at the microstructural level. Led by physicist Hector Lorenzana of the Laboratory's Defense and Nuclear Technologies Directorate, the team is probing, in real time, the lattice response of metals under high shock loads. Two diagnostic techniques—dynamic x-ray diffraction and synchrotron-based x-ray scattering—are being used to measure dynamic processes with nanometer and nanosecond resolutions. By combining these experimental data with high-performance computer simulations of material dynamics, the team can better understand how a material's crystalline lattice responds to extreme pressure.

Contact:

Hector Lorenzana (925) 422-8982 (lorenzana1@llnl.gov).

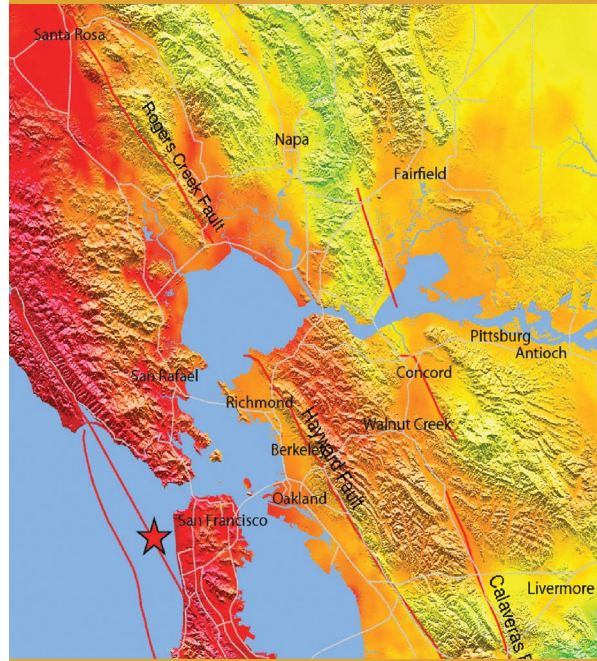
Planets and Stars under the Magnifying Glass

In 2005, an international collaboration of astronomers working with telescope networks throughout the Southern Hemisphere uncovered clues to a small Earth-like planet made of rock or ice. The new planet, designated OGLE-2005-BLG-290-Lb, is the farthest planet from our solar system detected to date. The discovery was made by PLANET, the Probing Lensing Anomalies Network, using microlensing—a technique developed nearly two decades ago by Lawrence Livermore scientists as part of the Massively Compact Halo Object (MACHO) Project, which searched for evidence of dark matter.

Contact:

Kem Cook (925) 423-4634 (cook12@llnl.gov).

Modeling the Big One



On the centennial of the 1906 San Francisco earthquake, Lawrence Livermore seismic experts revealed the most accurate simulations of the great quake ever conducted.

Also in September

- *New Livermore techniques may help identify the source of pathogens in a bioterrorist attack.*
- *A team of researchers from Livermore and the University of California investigate the role inelastic buckling plays in vertebral fracture of aging bone.*
- *Recent advances in precision manufacturing allow the production of double-shell targets with submicrometer tolerances for fusion experiments.*

Coming Next Month

University of California
Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

NONPROFIT ORG.
U.S. POSTAGE
PAID
LIVERMORE, CA
PERMIT NO. 154



Printed on recycled paper.